Investigation into Gaussian Quadrature

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1 Introduction

Quadrature is the name given to various methods used to approximate integrals. Some integrals are impossible or unfeasible to compute analytically (such as $\int e^{x^2}$), which necessitates the need to approximate them numerically. Thus, various methods have been developed to approximate these integrals, such as the Trapezoid Rule, Simpson's Rule, and Gaussian Quadrature. The aforementioned quadratures have varying levels of necessary computation and error. We intend to investigate and compare these quadrature forms. In particular, we will analyze the accuracy of Gaussian Quadrature to the more simple Trapezoid Rule and Simpson's Rule. Additionally, we will compare the theory of Guassian Quadrature convergence to experimental convergence.

2 Quadrature Techniques

2.1 Trapezoid Rule

The Trapezoid Rule is developed using Lagrange polynomials and equally spaced nodes. Consider $\int_a^b f(x)dx$. When we replace $f(x)$ with the first Lagrange polynomial approximation, with $x_0 = a$ and $x_1 = b$, and integrate, we get

$$\frac{(x_1 - x_0)}{2}[f(x_0) + f(x_1)] - \frac{(x_1 - x_0)^3}{12} f''(\xi)$$

Where $\xi \in (x_0, x_1)$. Naturally, we can set $h = x_1 - x_0$, resulting in the Trapezoid Rule:

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi)$$

It is clear that this approach only works well on quite small intervals; so, we develop the Composite Trapezoid Rule. The Composite Trapezoid Rule applies the Trapezoid Rule on n subintervals within the initial interval. The formula is as follows:

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{2}[f(x_0) + 2\sum_{j=1}^{n-1} f(x_j) + f(x_n)] - \frac{x_n - x_0}{12} h^2 f''(\mu)$$

Where $\mu \in (x_0, x_n)$.

2.2 Simpson's Rule

Similar to the Trapezoid Rule, Simpson's Rule is also developed using Lagrange polynomials. Simpson's Rule differs in that it uses the second Lagrange polynomial. Consider $\int_a^b f(x)dx$. We set $x_0 = a$, $x_1 = a + h$, and $x_2 = b$, where $h = \frac{b-a}{2}$. Now, when we replace $f(x)$ with the second Lagrange polynomial approximation and integrate, we get Simpson's Rule:

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi)$$

Where $\xi \in (x_0, x_2)$. However, like the Trapezoid Rule, this form only works well on small intervals. The Composite Simpson's Rule is developed similarly to the Composite

Trapezoid Rule, splitting the interval into n subintervals, where n is an even integer. The formula is as follows:

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{3}[f(x_0) + 2\sum_{j=1}^{\frac{n}{2}-1} f(x_{2j}) + 4\sum_{j=1}^{\frac{n}{2}} f(x_{2j-1}) + f(x_n)] - \frac{x_n - x_0}{180}h^4 f^{(4)}(\mu)$$

Where $\mu \in (x_0, x_n)$.

2.3 Guassian Quadrature

Gaussian quadrature is particularly efficient for integrating polynomials and uses specially chosen points and weights to achieve high accuracy.

Gaussian quadrature approximates integrals using:

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

where x_i are the nodes and w_i are the weights. The nodes and weights are chosen such that the method is exact for polynomials of degree $2n-1$ or lower. Typically, this integral is from $[-1, 1]$.

2.3.1 Motivation

Consider the trapezoid rule, which only provide exact solutions to integrals for linear functions. But we can do better, take n nodes $x_1, x_2, \cdots, x_n$. We can improve the trapezoid by choosing the weights such that they are exact for linear, quadratic, cubic, up to polynomials of degree $n-1$.

$$\int_{-1}^{1} f \approx w_1 f(x_1) + w_2 f(x_2) + \cdots + w_n f(x_n) \tag{1}$$

$$\begin{aligned}
f(x) = 1 &\rightarrow \int_{-1}^{1} 1\,dx = 2 = w_1 + w_2 + \cdot + w_n \\
f(x) = x &\rightarrow \int_{-1}^{1} x\,dx = 0 = w_1 x_1 + w_2 x_2 + \cdot + w_n x_n \\
&\vdots \\
f(x) = x^{n-1} &\rightarrow \int_{-1}^{1} x^{n-1}\,dx = 0 = w_1 x_1^{n-1} + w_2 x_2^{n-1} + \cdots + w_n x_n^{n-1}
\end{aligned}$$

Resulting in the following linear equation (with a Vandermonde Matrix):

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & \ddots & \cdots & x_n \\ \vdots & & \ddots & \\ x_1^{n-1} & x_2^{n-1} & \cdots & x_n^{n-1} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ \vdots \\ b_i \end{bmatrix}$$

In practice, this method is not feasible because Vandermonde matrices are badly ill-conditioned, as the condition number increases exponentially, (https://arxiv.org/abs/1504.02118), resulting in slight changes in b causing large changes in w_i's.

2.3.2 Derivation

We develop the formula for Gaussian quadrature using Legendre Polynomials - a series of orthogonal polynomials obtained by performing the Gram-Schmidt process on the standard basis for polynomials of degree n and the inner product $\langle p, q\rangle = \int_{-1}^{1} p(x)q(x)\,dx$. The first few Legendre Polynomials are as follows:

$$\begin{aligned} L_0(x) =& 1 \\ L_1(x) =& x \\ L_2(x) =& \frac{1}{2}(3x^2 - 1) \\ & \vdots \end{aligned}$$

Note that $L_i(x)$ is orthogonal to all polynomials of degree less than i, meaning $\forall p \in \mathbb{P}$, $\langle L_i, p\rangle$ for $\deg(p) \leq i$. Importantly, they also have exactly n roots over $\mathbb{R}$.

Now, given a polynomial $p(x)$ of degree $2n-1$, we can divide it by L_n, resulting in the following division with degrees:

$$\overbrace{p(x)}^{2n-1} = \overbrace{q(x)}^{n-1}\,\overbrace{L_n(x)}^{n} + \overbrace{r(x)}^{n-1} \tag{2}$$

Integrating both sides, we get

$$\int_{-1}^{1} p(x)\,dx = \int_{-1}^{1} q(x)L_n(x)\,dx + \int_{-1}^{1} r(x)\,dx = 0 + \int_{-1}^{1} r(x)\,dx$$

because the orthogonality of $L_n(x)$.
Going back to quadrature, we can ensure the same behavior by picking nodes at the zeros of $L_n(x)$.
Because $\int_{-1}^{1} p(x)\,dx = \int_{-1}^{1} r(x)\,dx$, we can interpolate $r(x)$ exactly with Lagrange polynomials, resulting in

$$\int_{-1}^{1} r(x)\,dx = \int_{-1}^{1} \left(\sum_{i=1}^{n} f(x_i)l_i(x)\right)\,dx = \sum_{i=1}^{n} f(x_i)\int_{-1}^{1} l_i(x)\,dx$$

meaning we choose our weights the be the integral of the Lagrange basis polynomials, or

$$w_i = \int_{-1}^{1} \prod_{j=1 j\neq i}^{n} \frac{x - x_j}{x_i - x_j}\,dx$$

This results in perfect interpolation of polynomials of degree $2n-1$, with n nodes. We can relate Lagrange and Legendre polynomials and then use the Christoffel-Darboux formula to rewrite the definition of the weights as

$$w_i = \frac{2}{(1 - x_i^2)(L_n'(x_i))^2} \tag{3}$$

Before using Gaussian Quadrature on any function, one must change an integral over $[a, b]$ to one over $[-1, 1]$. This can be done with

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{a+b}{2}\right)\frac{b-a}{2}\,dx$$

Resulting in a formula of:

$$\int_a^b f(x) \approx \frac{b-a}{2} \sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right) \tag{4}$$

3 Comparison of Quadrature

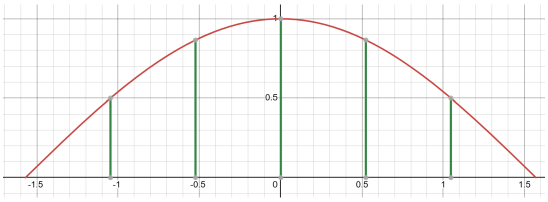

Figure 1: Simpson and Trapezoid, evenly spacing for $\cos x$

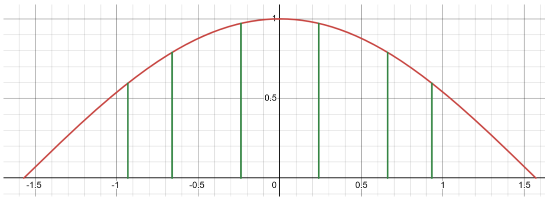

Figure 2: Gauss-Legendre node spacing, for $\cos x$

We applied Trapezoid Rule, Simpson's Rule, and Gaussian Quadrature to a series of five functions for the purpose of analysing and comparing the approximations. For each quadrature and function, we calculated the difference between the approximation and the analytical solution, as well as the order of convergence. Below is a table of our results.

Function	Method	Final Absolute Error	Terminated Early	Order of Convergence
F1	Trapezoid Rule	3.88475×10^{-7}	No	Non-Polynomial
F1	Simpson's Rule	2.33869×10^{-5}	No	$O(n^{2.32})$
F1	Gaussian Quadrature	7.56489×10^{-6}	No	Non-Polynomial
F2	Trapezoid Rule	N/A	N/A	N/A
F2	Simpson's Rule	N/A	N/A	N/A
F2	Gaussian Quadrature	0.348133	No	$O(n^{0.79})$
F3	Trapezoid Rule	0.0015914	No	$O(n^{1.22})$
F3	Simpson's Rule	0.000641819	No	$O(n^{1.59})$
F3	Gaussian Quadrature	0.000938918	No	$O(n^{1.21})$
F4	Trapezoid Rule	6.51042×10^{-6}	No	$O(n^{1.69})$
F4	Simpson's Rule	3.77476×10^{-14}	No	$O(n^{5.66})$
F4	Gaussian Quadrature	0	$n = 14$	$O(n^{11.36})$
F5	Trapezoid Rule	0.000257028	No	$O(n^{1.70})$
F5	Simpson's Rule	-2.64288×10^{-8}	No	$O(n^{3.45})$
F5	Gaussian Quadrature	0	$n = 12$	$O(n^{13.02})$

Integrals:

F1: $f(x) = \dfrac{1}{1 + 1000(x - 0.5)^2}, \quad [0, 1]$

F2: $f(x) = \dfrac{1}{x}\sqrt{\dfrac{1+x}{1-x}} \ln\left(\dfrac{2x^2 + 2x + 1}{2x^2 - 2x + 1}\right), \quad [-1, 1]$

F3: $f(x) = \sqrt{|x|}, \quad [-1, 1]$

F4: $f(x) = \dfrac{1}{1 + x^2}, \quad [0, 1]$

F5: $f(x) = \cos(x), \quad [-\dfrac{\pi}{2}, \dfrac{\pi}{2}]$

4 Order of Convergence

Talking points:

Function 1, Order of convergence Trapezoid > Gauss > Simpsons (look at log graph) What does non-polynomial mean? The order of convergence of the function cannot be expressed in the form of $O(n^m)$, m some real number. Show figures (see data folder, open in MATLAB, screenshot)

Function 2, Trapezoid Rule and Simpson's Rule cannot be used to approximate the integral because of a divide by zero. Gauss does not use the function directly in such a way that there is a divide by zero issue. This also demonstrates a worst-case scenario when using Gauss - it's roughly linear.

Function 3, interesting for having Gauss be worse than Simpson's but still better than Trapezoid

Function 4, Gauss was really good; we got to within machine precision (2^52) when $n = 14$ - so there was no need to continue calculating.

5 Conclusion

6 References

1. ”https://www.math.umd.edu/ mariakc/AMSC466/LectureNotes/quadrature.pdf”, page 22 error estimates
2. Numerical Analysis, Richard L. Burden, J. Douglas Faires, etc.